

Quantum Adiabatic Optimization and Combinatorial Landscapes

V.N. Smelyanskiy

S. Knysh

R.D. Morris

RIACS Technical Report 03.14

December 2003

Quantum Adiabatic Optimization and Combinatorial Landscapes

V.N. Smelyanskiy, NASA

S. Knysh, QSS

R.D. Morris, RIACS

RIACS Technical Report 03.14

December 2003

In this paper we analyze the performance of the Quantum Adiabatic Evolution (QAE) algorithm on a variant of Satisfiability problem for an ensemble of random graphs parametrized by the ratio of clauses to variables, $\alpha = M/N$. We introduce a set of macroscopic parameters (landscapes) and put forward an ansatz of universality for random bit flips. We then formulate the problem of finding the smallest eigenvalue and the excitation gap as a statistical mechanics problem. We use the so-called annealing approximation with a refinement that a finite set of macroscopic variables (*verses* only energy) is used, and are able to show the existence of a dynamic threshold $\alpha = \alpha_c$, beyond which QAE should take an exponentially long time to find a solution. We compare the results for extended and simplified sets of landscapes and provide numerical evidence in support of our universality ansatz.

Quantum adiabatic optimization and combinatorial landscapes

V. N. Smelyanskiy,^{*} S. Knysh,[†] and R.D. Morris[‡]

NASA Ames Research Center, MS 269-3, Moffett Field, CA 94035-1000

(Dated: December 16, 2003)

In this paper we analyze the performance of the Quantum Adiabatic Evolution (QAE) algorithm on a variant of Satisfiability problem for an ensemble of random graphs parametrized by the ratio of clauses to variables, $\gamma = M/N$. We introduce a set of macroscopic parameters (landscapes) and put forward an ansatz of universality for random bit flips. We then formulate the problem of finding the smallest eigenvalue and the excitation gap as a statistical mechanics problem. We use the so-called annealing approximation with a refinement that a finite set of macroscopic variables (*verses* only energy) is used, and are able to show the existence of a dynamic threshold $\gamma = \gamma_d$, beyond which QAE should take an exponentially long time to find a solution. We compare the results for extended and simplified sets of landscapes and provide numerical evidence in support of our universality ansatz.

PACS numbers: 03.67.Lx, 89.70.+c

I. INTRODUCTION

An important open question in the field of quantum computing is whether it is possible to develop quantum algorithms capable of efficiently solving combinatorial optimization problems (COP). In the simplest case the task in a COP is to minimize the energy function E_σ with the domain given by the set of all possible assignments of N binary variables, $\sigma = \{\sigma_1, \dots, \sigma_N\}$, $\sigma_j = \pm 1$. In quantum computation this cost function corresponds to a Hamiltonian \mathcal{H}_P

$$\mathcal{H}_P = \sum_{\sigma} E_\sigma |\sigma\rangle \langle \sigma| \quad (1)$$
$$|\sigma\rangle = |\sigma_1\rangle_1 \otimes |\sigma_2\rangle_2 \otimes \dots \otimes |\sigma_N\rangle_N,$$

^{*}Electronic address: Vadim.N.Smelyanskiy@nasa.gov

[†]Electronic address: knysh@email.arc.nasa.gov

[‡]Electronic address: rdm@email.arc.nasa.gov

where the summation is over the 2^N states $|\sigma\rangle$ forming the computational basis of a quantum computer with N qubits. State $|\sigma_j\rangle_j$ of the j -th qubit is an eigenstate of the Pauli matrix $\hat{\sigma}_z$ with eigenvalue σ_j . It is clear from the above that the ground state of H_P encodes the solution to the COP with cost function E_σ . In what follows we shall use two equivalent notations for binary variables: Ising spins $\sigma_j = \pm 1$ as well as bits $z_j = (1 - \sigma_j)/2 = 0, 1$.

Recently Farhi and coworkers proposed a new family of quantum algorithms for combinatorial optimization that is based on the properties of quantum adiabatic evolution [1, 2]. Numerical simulations were performed for the study of its performance for satisfiability problems [8]. Implementation of these algorithms on a quantum computing device is feasible for COPs where the energy function E_σ possesses a locality property, in a sense that it is given by the sum of terms each involving only a relatively small number of bits, that does not scale with N [1, 3, 4]. An example of a problem that can have this property is Satisfiability that deals with N binary variables, submitted to M constraints, assuming that each constraint involves $\mathcal{O}(1)$ bits. The task is to find a bit assignment that satisfies all the constraints.

Satisfiability is a basic problem in the so-called NP-complete class [5]. This class contains hundreds of the most common computationally hard problems encountered in practice, such as constraint satisfaction and graph coloring. NP-complete problems are characterized in the worst case by exponential scaling of the run time or memory requirement with the problem size N . A special property of the class is that any NP-complete problem can be converted into any other NP-complete problem in polynomial time on a classical computer. Therefore, it is sufficient to find a deterministic algorithm that can be guaranteed to solve all instances of just one of the NP-complete problems within a polynomial time bound. It is widely believed, however, that such an algorithm does not exist on a classical computer. Whether it exists on a quantum computer is one of the central open questions.

Running of the quantum adiabatic evolution algorithms (QAA) for several NP-complete problems has been simulated on a classical computer using a large number of randomly generated problem instances that are believed to be computationally hard for classical algorithms [2, 6, 8]. Results of these numerical simulations for relatively small size of the problem instances ($N \lesssim 25$) suggest a *quadratic* scaling law of the run time of the QAA with N .

A particularly simple version of Satisfiability is the NP-complete Exact Cover problem that was used in [2] to study the performance of QAA. In this problem each constraint is a clause that involves a subset of $K = 3$ binary variables. A given constraint is satisfied if exactly one of its bits

equals 1 and the rest of the bits equal 0. In the optimization version of this problem one minimizes the energy function E_σ that is equal to the number of constraints violated by a given bit-assignment σ . A generalization of this problem to an arbitrary number K can be called positive 1-in-K SAT [9].

In practice algorithms for NP-complete problems are characterized by a wide range of running times, from linear to exponential, depending on the choice of certain control parameters of the problem (e.g., in Satisfiability it is the ratio of the number of constraints to the number of variables, M/N). Therefore, a practically important alternative to the worst case complexity analysis is study of a typical-case behavior of optimization algorithms on ensembles of randomly generated problem instances chosen from a given probability distribution. For example, in the case of positive 1-in-K SAT one can define a uniform ensemble of random problem instances. An instance \mathcal{I} consists of M statistically independent clauses, each corresponding to a K -tuple of distinct bit-indices uniformly sampled from the interval $(1, N)$ with probability $1/\binom{N}{K}$.

In the case of an exponential scaling law for the algorithm's running times t_a it is convenient to analyze the distribution of a normalized logarithmic quantity $\log t_a/N$. This distribution becomes increasingly narrow in the limit of large N where the mean value $\langle \log t_a \rangle/N$ well characterizes the typical case exponential complexity of an algorithm. For Satisfiability problem the dependence of the asymptotic quantity

$$\eta = \lim_{N \rightarrow \infty} \langle \log t_a \rangle / N \quad (2)$$

on the clause-to-variable ratio $\gamma = M/N$ has the qualitative form shown in Fig.1. At some critical value $\gamma = \gamma_d$ algorithmic complexity undergoes the dynamical transition from polynomial to exponential scaling law. This transition has been studied recently for the case of a variant of the classical random-walk algorithm for the Satisfiability problem [10]. Function $\eta(\gamma)$ is non-monotonic in γ and reaches its maximum at a certain point $\gamma_c > \gamma_d$. It was discovered some time ago [11, 13, 14] that γ_c is a critical value for the so called satisfiability phase transition: if $\gamma < \gamma_c$, a randomly drawn instance is satisfiable with high probability, i.e., there exists at least one bit assignment σ that satisfies all the constraints ($E_\sigma = 0$). For $\gamma > \gamma_c$ instances are almost never satisfiable. In the asymptotic limit $N \rightarrow \infty$ the proportion of satisfiable instances drops from 1 to 0 infinitely steeply at $\gamma = \gamma_c$ as shown in Fig. 1.

The value of γ_d (unlike γ_c) depends on both the problem at hand and the optimization algorithm. Comparison of the dynamical thresholds γ_d for different algorithms provides an important relative measure of their typical-case performance in a given problem. In this paper we will provide the

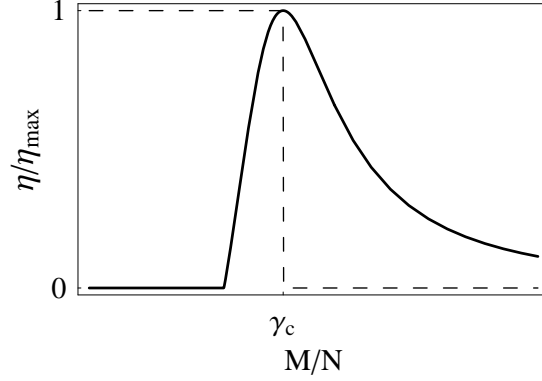


FIG. 1: Solid line shows the qualitative plot of the normalized quantity η/η_{\max} vs M/N (η_{\max} is a maximum value of η). Dashed line shows the proportion of satisfiable instances vs M/N .

analysis of the dynamical threshold for the quantum adiabatic evolution algorithm and also for simulated annealing for several versions of the random satisfiability problem.

II. QUANTUM ADIABATIC EVOLUTION ALGORITHM

Consider the time-dependent Hamiltonian $H(t) \equiv \mathcal{H}(t/T)$

$$\mathcal{H}(\tau) = (1 - \tau) \mathcal{H}_B + \tau \mathcal{H}_P, \quad (3)$$

where $\tau = t/T \in (0, 1)$ is dimensionless “time”, \mathcal{H}_P is the “problem” Hamiltonian (1) and \mathcal{H}_B is a “driver” Hamiltonian, that is designed to cause transitions between the eigenstates of \mathcal{H}_P . Using dimensionless time and setting $\hbar = 1$ the quantum state evolution obeys the equation, $i T \partial |\Psi(\tau)\rangle / \partial \tau = \mathcal{H}(\tau) |\Psi(\tau)\rangle$. At the initial moment the quantum state $|\Psi(0)\rangle$ is prepared to be the ground state of $\mathcal{H}(0) = \mathcal{H}_B$. In the simplest case

$$\mathcal{H}_B = - \sum_{j=1}^N \sigma_x^j, \quad |\Psi(0)\rangle = 2^{-N/2} \sum_{\sigma} |\sigma\rangle, \quad (4)$$

where σ_x^j is a Pauli matrix for j -th qubit. Consider the instantaneous eigenstates of $\mathcal{H}(\tau)$ with eigenvalues $\lambda_k(\tau)$ arranged in nondecreasing order at any value of $\tau \in (0, 1)$

$$\mathcal{H}(\tau) |\phi_k(\tau)\rangle = \lambda_k(\tau) |\phi_k(\tau)\rangle, \quad (5)$$

here $k = 0, 1, 2, \dots, 2^N - 1$. Provided the value of T (the runtime of the algorithm) is large enough and there is a finite gap for all $\tau \in (0, 1)$ between the ground and excited state energies,

$\lambda_1(\tau) - \lambda_0(\tau) > 0$, the quantum evolution is adiabatic and the state of the system $|\Psi(\tau)\rangle$ stays close to an instantaneous ground state, $|\phi_0(\tau)\rangle$ (up to a phase factor). The state $|\phi_0(1)\rangle$ coincides with the ground state of the problem Hamiltonian \mathcal{H}_P and, therefore, a measurement performed on the quantum computer at the final moment $t = T$ ($\tau = 1$) will yield one of the solutions of COP with large probability.

The standard criterion for adiabatic evolution is usually formulated in terms of minimum excitation gap between the ground and first excited states [12]

$$T \gg \frac{\mathcal{E}}{\Delta\lambda_{\min}^2}, \quad \Delta\lambda_{\min} = \max_{0 \leq \tau \leq 1} [\lambda_1(\tau) - \lambda_0(\tau)]. \quad (6)$$

Here the quantity \mathcal{E} is less than the largest eigenvalue of the operator $\mathcal{H}_P - \mathcal{H}_B$ [18] and scales polynomially with N in the problems we consider.

III. QUASICLASSICAL APPROXIMATION AND COMBINATORIAL LANDSCAPES

In the computational basis (1) we have

$$\mathcal{H} = \tau \sum_{\sigma} E_{\sigma} |\sigma\rangle\langle\sigma| - (1 - \tau) \sum_{\sigma, \sigma'} \delta[d(\sigma, \sigma'), 1] |\sigma\rangle\langle\sigma'|, \quad (7)$$

here $\delta[m, n]$ denotes the Kronecker delta-symbol and the summation is over the pairs of spin configurations σ and σ' that differ by the orientation of a single spin, $d(\sigma, \sigma')=1$, where

$$d(\sigma, \sigma') = \frac{1}{2} \sum_{j=1}^N |\sigma_j - \sigma'_j|, \quad (8)$$

denotes a so-called Hamming distance between the spin configurations σ and σ' , that is the number of spins with opposite orientations. Eq. (5) in the computational basis takes form

$$\lambda(\tau)\phi_{\sigma}(\tau) = \tau E_{\sigma}\phi_{\sigma}(\tau) - (1 - \tau) \sum_{\sigma'} \delta[d(\sigma, \sigma'), 1] \phi_{\sigma'}(\tau) \quad (9)$$

(here we drop the subscript indicating the number of a quantum state in λ and ϕ_{σ}). In what follows we assume that typical energies $E_{\sigma} = \mathcal{O}(N)$, but the change in the energy after a single spin flip is $\mathcal{O}(1)$. This assumption about the energy landscape holds for instances of the Satisfiability problem with the clause-to-variable ratio $M/N = \mathcal{O}(1)$, the case of most interest for us (see the discussion in Sec. I).

We now consider a set of functions $\{X_l = C_l(\sigma, \mathcal{I}), l = 1, \dots, \mathcal{K}\}$, referred to as (combinatorial) landscapes, that depend on a problem instance \mathcal{I} and project a spin configuration σ

onto a vector $\{X_l\}$ with integer-valued components. Prior to considering a specific COP here we make certain assumptions about the properties of landscapes and apply them to the analysis of the minimum gap in the QAA.

In particular, we assume that, similar to energy, landscapes $\{X_l = C_l(\boldsymbol{\sigma}, \mathcal{I})\}$ are macroscopic functions, so that the typical values of X_l are $\mathcal{O}(N)$, and possess a certain *universality* property in the asymptotic limit $N \rightarrow \infty$. Specifically, the joint distribution of $\{C_l(\boldsymbol{\sigma}, \mathcal{I})\}$ over the spin configurations $\boldsymbol{\sigma}$ forming the 1-spin-flip neighborhood of an “ancestor” configuration $\boldsymbol{\sigma}'$ depends on a problem instance \mathcal{I} and spin configuration $\boldsymbol{\sigma}'$ *only* via the set of parameters $\{X'_l = C_l(\boldsymbol{\sigma}', \mathcal{I})\}$. We then define a quantity

$$P(\{X_l\} | \{X'_l\}) = \frac{1}{N} \sum_{d(\boldsymbol{\sigma}, \boldsymbol{\sigma}')=1} \prod_{k=1}^{\kappa} \delta[X_l, C_l(\boldsymbol{\sigma}, \mathcal{I})], \quad (10)$$

$$X'_l = C_l(\boldsymbol{\sigma}', \mathcal{I}),$$

In effect, the above universality property of landscapes implies that the set of all possible spin configurations $\boldsymbol{\sigma}$ is divided into “boxes” with coordinates $\{X_l\}$ where $X_l = C_l(\boldsymbol{\sigma})$, and $P(\{X_l\} | \{X'_l\})$ (10) represents the transition probability from box $\{X_l\}$ to box $\{X'_l\}$. In particular, it obeys Bayes’ rule

$$P(\{X_l\} | \{X'_l\}) \Omega(\{X'_l\}) = P(\{X'_l\} | \{X_l\}) \Omega(\{X_l\}), \quad (11)$$

where $\Omega(\{X_l\})$ is the number of different spin configurations in the box $\{X_l\}$.

We consider energy to be a smooth function of landscapes

$$E_{\boldsymbol{\sigma}} = E(\{X_l\}), \quad X_l \equiv C_l(\boldsymbol{\sigma}, \mathcal{I}), \quad (12)$$

so that $|\partial E / \partial X_l| = \mathcal{O}(1)$. Furthermore, we assume that, on one hand, the change in $C_l(\boldsymbol{\sigma}, \mathcal{I})$ after flipping one spin is $\mathcal{O}(1)$, for typical problem instances. On the other hand, we assume that correlation properties in a neighborhood of a box $\{X_l\}$ described by $P(\{X_l\} | \{X'_l\})$ vary smoothly with box coordinates on a scale $1 \lesssim |\delta X_l| \ll N$. Therefore if we write the transition probability in the form

$$P(\{X'_l\} | \{X_l\}) = p(\{X'_l - X_l\}; \{x_l\}), \quad \{x_l \equiv X_l/N\}, \quad (13)$$

then $p(\{k_l\}; \{x_l\})$ is a steep function of its first argument: it decays rapidly in the range $1 \lesssim |k_l| \ll N$ for each l -component. However this is a smooth function of its second argument: it varies slightly when coordinates x_l change on a scale $|\delta x_l| \ll 1$.

One can show that under the above assumptions the quantum amplitudes ϕ_{σ} corresponding to the smallest eigenvalue depend on the spin configuration σ only via the coordinates of the box $\{X_l\}$ to which it belongs. Then we look for the solution of (9) in the following form:

$$\phi_{\sigma}(\tau) = \frac{\varphi(\{X_l\}, \tau)}{\sqrt{\Omega(\{X_l\})}}, \quad \{X_l \equiv C_l(\sigma, \mathcal{I})\}. \quad (14)$$

where $|\varphi(\{X_l\}, \tau)|^2$ gives the probability of finding the system in the box $\{X_l\}$. Plugging (14) into (9) and making use of (11),(12) we obtain:

$$\lambda(\tau)\varphi(\mathbf{X}, \tau) = \tau E(\mathbf{X})\varphi(\mathbf{X}, \tau) - (1 - \tau)N \sum_{\mathbf{X}'} L(\mathbf{X}, \mathbf{X}') \varphi(\mathbf{X}', \tau), \quad (15)$$

$$\mathbf{X} \equiv \{X_1, X_2, \dots, X_K\}, \quad (16)$$

(hereafter we use the above shorthand notation for the set of landscapes). In (15) we introduced **L**

$$L(\mathbf{X}, \mathbf{X}') = L(\mathbf{X}', \mathbf{X}) = P(\mathbf{X}'|\mathbf{X}) \sqrt{\frac{P(\mathbf{X})}{P(\mathbf{X}')}}, \quad (17)$$

$$P(\mathbf{X}) = 2^{-N} \Omega(\mathbf{X}),$$

where $P(\mathbf{X})$ is a probability that a randomly sampled configuration σ belongs to a box \mathbf{X} . We shall look for a solution of (15) in the WKB-like form

$$\varphi(\mathbf{X}, \tau) = \exp(-W(\mathbf{X}, \tau)), \quad (18)$$

so that

$$\lambda(\tau) = \tau E(\mathbf{X}) - (1 - \tau)N \sum_{\mathbf{X}'} L(\mathbf{X}, \mathbf{X}') e^{W(\mathbf{X}, \tau) - W(\mathbf{X}', \tau)}. \quad (19)$$

We now introduce scaled variables (cf. (13))

$$\mathbf{x} = \frac{\mathbf{X}}{N}, \quad \Gamma = \frac{1 - \tau}{\tau}, \quad g = \frac{\lambda}{\tau N}, \quad (20)$$

and also

$$w(\mathbf{x}, \Gamma) \equiv \frac{1}{N} W(\mathbf{X}, \tau), \quad \varepsilon(\mathbf{x}) \equiv \frac{1}{N} E(\mathbf{X}), \quad s(\mathbf{x}) \equiv \frac{1}{N} \log \Omega(\mathbf{X}), \quad (21)$$

where $s(\mathbf{x})$ is an entropy function. Based on (17) and the properties of the transition probability (see Eq. (13) and discussion after it) we assume that the sum over \mathbf{X}' in (19) is dominated by terms with $|\mathbf{X}' - \mathbf{X}| = \mathcal{O}(1)$. Then we can use an approximation

$$W(\mathbf{X}', \tau) - W(\mathbf{X}, \tau) \approx \nabla w \cdot (\mathbf{X}' - \mathbf{X}) + \mathcal{O}(1/N), \quad (22)$$

where $\nabla w \equiv \partial w(\mathbf{x}, \Gamma)/\partial \mathbf{x}$. Plugging (22) into (19) and making use of Eqs. (13),(17),(20) and (21) we obtain after some transformations:

$$\begin{aligned} g &= h(\mathbf{x}, \nabla w; \Gamma), \\ h(\mathbf{x}, \mathbf{p}; \Gamma) &= \varepsilon(\mathbf{x}) - \Gamma \sum_{\mathbf{k}} p(\mathbf{k}; \mathbf{x}) e^{-\mathbf{k} \cdot (\nabla s/2 + \mathbf{p})}. \end{aligned} \quad (23)$$

(here $\nabla s \equiv \partial s(\mathbf{x})/\partial \mathbf{x}$). This is a Hamilton-Jacobi equation for an auxiliary mechanical system with coordinates \mathbf{x} , momenta $\mathbf{p} = \nabla w$, action w , Hamiltonian function $h(\mathbf{x}, \mathbf{p}; \Gamma)$ and energy g . Using the symmetry relation

$$p(\mathbf{k}; \mathbf{x}) e^{-\mathbf{k} \cdot \nabla s/2} = p(-\mathbf{k}; \mathbf{x}) e^{\mathbf{k} \cdot \nabla s/2}, \quad (24)$$

that follows directly from Eqs. (11) and (17) we obtain that the minimum of $w(\mathbf{x}, \Gamma)$ over \mathbf{x} where $\nabla w = 0$ necessary corresponds to the minimum of the functional:

$$f(\mathbf{x}, \Gamma) = \varepsilon(\mathbf{x}) - \Gamma \ell(\mathbf{x}), \quad (25)$$

where $f(\mathbf{x}, \Gamma) \equiv h(\mathbf{x}, \mathbf{0}, \Gamma)$ and

$$\ell(\mathbf{x}) = \tilde{p}(\nabla s/2; \mathbf{x}), \quad \tilde{p}(\mathbf{y}; \mathbf{x}) \equiv \sum_{\mathbf{k}} p(\mathbf{k}; \mathbf{x}) e^{-\mathbf{k} \cdot \mathbf{y}}. \quad (26)$$

The summation in (23) and (26) is over components k_l of \mathbf{k} in the range $k_l \in (-\infty, \infty)$. In what follows, we shall refer to $\tilde{p}(\mathbf{y}; \mathbf{x})$ in (26) as a ‘‘Laplace transform’’ of $p(\mathbf{k}; \mathbf{x})$.

We note that $\ell(\mathbf{x}) = \sum_{\mathbf{X}'} L(\mathbf{X}', \mathbf{X})$ and one can use Bayes rule and inequality of Cauchy-Bunyakovsky in (17) to show that the positive-valued function $\ell(\mathbf{x})$ is bounded from above, $0 < \ell(\mathbf{x}) \leq 1$. This shows that the analysis of the effective potential based on the WKB approximation (22) is self-consistent in the asymptotic limit $N \rightarrow \infty$.

It follows from the above analysis that the ground-state wavefunction $\psi(\mathbf{x}, \Gamma) \equiv \varphi(\mathbf{X}, \tau)$ is concentrated in \mathbf{x} -space near the bottom of the ‘‘effective potential’’ given by the functional $f(\mathbf{x}, \Gamma)$, i.e. near the point $\mathbf{x}_*(\Gamma)$ where $f(\mathbf{x}, \Gamma)$ reaches its minimum. In this region $S \approx \frac{1}{2} \mathbf{x}^T \hat{\mathbf{A}} \mathbf{x}$, where matrix $\hat{\mathbf{A}}$ is positive definite, and according to (18), the wavefunction has a Gaussian form with the width $\propto 1/\sqrt{N}$.

The ground-state energy $g \equiv g(\Gamma)$ is given by the value of the effective potential f (25) at its minimum

$$\begin{aligned} g(\Gamma) &= f(\mathbf{x}_*(\Gamma), \Gamma), \\ \partial f(\mathbf{x}, \Gamma)/\partial \mathbf{x}|_{\mathbf{x}=\mathbf{x}_*(\Gamma)} &= 0, \quad f(\mathbf{x}, \Gamma) \geq g(\Gamma). \end{aligned} \quad (27)$$

We note that as $\Gamma \rightarrow 0$ the shape of the effective potential $f(\mathbf{x}, \Gamma)$ approaches that of the energy function $\varepsilon(\mathbf{x})$ and therefore its minimum $\mathbf{x}_*(\Gamma) \rightarrow \mathbf{x}_0$ where \mathbf{x}_0 is a minimum of $\varepsilon(\mathbf{x})$. It can be shown that in this limit the ground-state eigenvalue approaches the minimum energy value $\varepsilon(\mathbf{x}_0)$ and the eigenvalues of \mathbf{A}^{-1} approach zero (and so does the characteristic width of the wavepackage $\psi(\mathbf{x}, \Gamma)$). The spin configurations that belong to a box \mathbf{x}_0 in \mathbf{x} -space correspond to the solutions of the optimization problem at hand. It is clear that one of the solutions can be recovered with high probability after a measurement is performed at the end of the “quantum annealing” procedure.

Variational Ansatz: For cases in which the set of macroscopic variables $\{X_l\}$ is not sufficient (in statistical sense (13)) to describe the dynamics of the quantum algorithm, one can still implement the above procedure as an *approximation*, using a variational method. Introducing a Lagrangian multiplier λ , one looks for the minimum of the functional $F(\varphi, \lambda) = \langle \phi | \mathcal{H} | \phi \rangle - \lambda(\langle \phi | \phi \rangle - 1)$, using a variational ansatz (14) for the wavefunction. The solution of the variational problem is provided by Eqs. (18)-(27). The smallest eigenvalue g (27) corresponds to the value of the Lagrange multiplier at the extremum, $\lambda = \tau N g$, and the maximum of the variational wavefunction corresponds to the minimum of the effective potential f (25).

A. Global bifurcations of the effective potential

However, in the case of a global bifurcation where the effective potential $f(\mathbf{x}, \Gamma)$ possesses degenerate or nearly degenerate global minima, the answer is modified. If for some value of $\Gamma = \Gamma_*$, a global bifurcation occurs, in our example this would mean that for this value of Γ , two values of \mathbf{x} , \mathbf{x}_*^+ and \mathbf{x}_*^- give a global minimum to $f(\mathbf{x}, \Gamma)$. In such a case, the smallest eigenvalue is not doubly degenerate; rather an exponentially small gap $\Delta\lambda_{\min}$ between the ground and first excited state is developed, itself being proportional to the overlap between two wave-functions, peaked around \mathbf{x}_*^+ and \mathbf{x}_*^- respectively.

To estimate the overlap we note that at Γ_* the two global minima of the effective potential $f(\mathbf{x}, \Gamma_*)$ correspond to the two coexisting fixed points of the Hamiltonian function in (23) with zero momentum and the same values of energy g ,

$$\partial f / \partial \mathbf{x} = \partial h / \partial \mathbf{x} = \partial h / \partial \mathbf{p} = 0 \quad (28)$$

$$\mathbf{x} = \mathbf{x}_*^\pm, \quad \mathbf{p} = \mathbf{p}_*^\pm = 0, \quad g(\mathbf{x}, \mathbf{p}; \Gamma_*) = g_*^+ = g_*^-. \quad (29)$$

Then to logarithmic accuracy we have

$$\frac{1}{N} \log \Delta g_{\min} = \int_{-\infty}^{\infty} dt' [\dot{\mathbf{x}}(t') \mathbf{p}(t') - h(\mathbf{x}(t'), \mathbf{p}(t'))] + \mathcal{O}(1/N), \quad (30)$$

where $(\mathbf{x}(t), \mathbf{p}(t))$ is a heteroclinic trajectory connecting the two fixed points of (23)

$$\begin{aligned} \dot{\mathbf{x}}(t) &= \partial h / \partial \mathbf{p}, \quad \dot{\mathbf{p}}(t) = -\partial h / \partial \mathbf{x}, \\ \mathbf{x}(t \rightarrow \pm\infty) &= \mathbf{x}_*^{\pm}, \quad \mathbf{p}(t \rightarrow \pm\infty) = 0. \end{aligned} \quad (31)$$

From the algorithmic perspective this means that when Γ gets close to Γ_* , it has to change exponentially slowly (cf. Sec. II and Eq. (6)). This could be called a critical slowing down in the vicinity of a quantum phase transition. If simulated annealing (SA) is used and a similar phenomenon occurs, the value of the temperature T_* is the point where a global bifurcation occurs in the free energy functional

$$f(\mathbf{x}, T) = \varepsilon(\mathbf{x}) - Ts(\mathbf{x}). \quad (32)$$

By comparing the free energy functional (32) with the functional (25) corresponding to “quantum annealing” (QA), we note that in QA the quantities Γ and $\ell(\mathbf{x})$ play the roles of temperature and entropy in (SA), respectively.

We note in passing that a similar picture for the onset of global bifurcation that can lead to the failure of QA and (or) SA was proposed in [18, 19] for the case where the energy E_{σ} is a non-monotonic function of a single landscape parameter, a total spin $\sum_{j=1}^N \sigma_j$. In this case the dynamics of QA can be described in terms of one-dimensional effective potential [20, 23].

IV. THE MODELS

An instance of a Satisfiability problem with N binary variables committed to $M = \gamma N$ constraints (where each constraint is a clause involving K variables) can be defined by the specification of the following two objects. One of them is an $M \times N$ matrix $\hat{\mathcal{G}}$, the rows of the matrix are independent K -tuples of distinct bit indexes sampled from the interval $(1, N)$. The m -th row of $\hat{\mathcal{G}}$ defines the subset of the K binary variables involved in the m -th clause. The second object is a set of boolean functions $\mathcal{B} = \{b_m\}$, with each function encoding a corresponding constraint. A function $b_m = b_m[\sigma_{g_{m1}}, \sigma_{g_{m2}}, \dots, \sigma_{g_{mK}}]$ is defined over the set of 2^K possible assignments of the string of K binary variables involved in the m -th clause. The function returns value 1 for

assignments of binary variables that satisfy the constraint and 0 for bit assignments that violate it. Then the energy function equals to the number of violated constraints

$$E_{\sigma} \equiv E_{\sigma}(\mathcal{I}) = M - \sum_{m=0}^M b_m[\sigma_{g_{m1}}, \sigma_{g_{m2}}, \dots, \sigma_{g_{mK}}], \quad (33)$$

here $\mathcal{I} = (\mathcal{G}, \mathcal{B})$ denotes an instance of a problem.

The matrix $\hat{\mathcal{G}}$ defines a hypergraph \mathcal{G} that is made up of the set of N vertices (corresponding to the variables in the problem) and a set of M hyperedges (corresponding to the constraints of the problem), each one connecting K vertices. An ensemble of *disorder configurations* of the hypergraph corresponds to all the possible ways one can place $M = \gamma N$ hyperedges among N vertices where each hyperedges carries K vertices. Under the uniformity ansatz all configurations of disorder are sampled with equal probabilities (i.e., rows of the matrix $\hat{\mathcal{G}}$ are independently and uniformly sampled in the $(1, N)$ interval).

Boolean functions b_m may also be generated at random for each constraint with an example being random K-SAT problem [16, 17]. However here we consider slightly different versions of the random Satisfiability problem that are still defined on a random hypergraph \mathcal{G} but have a non-random boolean function $b_m = b$, identical for all the clauses in a problem. One of the problems is Positive 1-in-K Sat in which a constrain is satisfied if and only if exactly one bit is equal 1 and the other $K-1$ bits are equal 0. The boolean function b for this problem takes the form

$$b[\alpha_1, \alpha_2, \dots, \alpha_K] = \delta \left[\sum_{p=1}^K \frac{1 - \alpha_p}{2}, 1 \right] \quad (\text{Positive 1-in-K Sat}). \quad (34)$$

$$\alpha_p = \pm 1, \quad p = 1, 2, \dots, K.$$

We shall also consider another problem, Positive K-NAE-Sat, in which a clause is satisfied unless all variables that appear in a clause are equal ("K-Not-All-Equal-Sat"). The boolean function b for this problem takes the form

$$b[\alpha_1, \alpha_2, \dots, \alpha_K] = 1 - \sum_{s=\pm 1} \delta \left[\sum_{p=1}^K \frac{1 + s \alpha_p}{2}, 0 \right] \quad (\text{Positive K-NAE-Sat}). \quad (35)$$

Both problems are NP-complete (Appendix A). It will be shown below that they are characterized by the same set of landscape functions.

V. LANDSCAPES: ANNEALING APPROXIMATION

For a particular spin (σ) and disorder (\mathcal{G}) configurations, all clauses can be divided into 2^K distinct groups according to the values of the binary variables that appear in a clause. We will label the different types of clauses by vectorial index $\alpha = \{\alpha_1, \dots, \alpha_K\}$, $\alpha_p = \pm 1$. We now divide the set of 2^N spin configurations into boxes identified by certain numbers of clauses of each type, $N M_\alpha$, and also by the Ising spin in a configuration Nq

$$M_\alpha \equiv M_\alpha(\sigma, \mathcal{G}) = \frac{1}{N} \sum_{m=1}^M \prod_{p=1}^K \delta[\sigma_{\mathcal{G}_{mp}}, \alpha_p], \quad (36)$$

$$q \equiv q(\sigma) = \frac{1}{N} \sum_{j=1}^N \sigma_j. \quad (37)$$

Different boxes correspond to macroscopic states defined by the set of parameters $(q, \{M_\alpha\})$ with $q \in (-1, 1)$ and $\sum_\alpha M_\alpha = \gamma$. The energy function can be expressed via (36) as follows (cf. (33)-(35)):

$$\varepsilon(\{M_\alpha\}) = \gamma - \sum_{m=0}^K \zeta_m \mathcal{M}_m, \quad \mathcal{M}_m \equiv \sum_\alpha M_\alpha \delta\left[K - 2m, \sum_{p=1}^K \alpha_p\right], \quad (38)$$

where the form of the coefficients ζ_m depends on the problem:

$$\zeta_m = \begin{cases} \delta[m, 1] & \text{(Positive 1-in-K Sat)} \\ 1 - \delta[m, 0] - \delta[m, K] & \text{(Positive K-NAE-Sat)} \end{cases} \quad (39)$$

In the following we compute an approximation to the effective potential (25), using the landscape functions (36), (37). According to (26) it depends on the entropy function $s(q, \{M_\alpha\})$ and the transition probability (13) between different macroscopic states. Recalling that variables q and M_α are normalized by the factor N we study the probability of transition, $p(n, \{r_\alpha\}; q, \{M_\alpha\})$, from the state $(q, \{M_\alpha\})$ to the state $(q + n/N, \{M_\alpha + r_\alpha/N\})$. The Laplace transform of p with respect to $n, \{r_\alpha\}$ has the form (cf. (26))

$$\tilde{p}(\theta, \{y_\alpha\}; q, \{M_\alpha\}) = \sum_{n, \{r_\alpha\}} e^{-\theta n - \sum_\alpha y_\alpha r_\alpha} p(n, \{r_\alpha\}; q, \{M_\alpha\}), \quad (40)$$

We assume that all binary variables are also subdivided into distinct groups based on their value $\sigma = \pm 1$ and a vector \mathbf{k} with integer coefficients k_α^p indicating the number of times a variable appears in a clause of type α in position p . Clearly, consistency requires that $k_\alpha^p = 0$ unless

$\alpha_p = \sigma$. We now define a quantity $c_{\sigma,\mathbf{k}}$ which is equal to the fraction of spins with given σ, \mathbf{k} . For a spin configuration σ there exists a set of coefficients $\{c_{\sigma,\mathbf{k}}\}$ with elements of the set corresponding to all possible values of σ and \mathbf{k} (there will be many 0's in a set for each spin configuration). In general, there are exponentially many sets $\{c_{\sigma,\mathbf{k}}\}$ that correspond to a macroscopic state $(q, \{M_\alpha\})$

$$\sum_{\sigma,\mathbf{k}} \sigma c_{\sigma,\mathbf{k}} = q, \quad \sum_{\sigma,\mathbf{k}} k_\alpha^p c_{\sigma,\mathbf{k}} = M_\alpha \quad (p = 0, 1, \dots, K). \quad (41)$$

Coefficients $\{c_{\sigma,\mathbf{k}}\}$ are concentrations of spin variables with different types of “neighborhoods”. We shall assume that in the limit of large N the distribution of coefficients $c_{\sigma,\mathbf{k}}$ corresponding to the same macroscopic state (41) is sharply peaked around their mean values (with the width of the distribution $\propto N^{-1/2}$).

Under the above assumption we can immediately compute the Laplace-transformed transition probability (40) in terms of the coefficients $c_{\sigma,\mathbf{k}}$. Indeed, consider flipping a spin with value σ and neighborhood type given by vector \mathbf{k} . This will change the total spin by -2σ and for each clause of type α and index $p \in (1, K)$ the value of NM_α will decrease by k_α^p . On the other hand, for the clause type $\alpha' \equiv \bar{\alpha}(p, \alpha)$ obtained by flipping a bit in p -th position in α , $NM_{\alpha'}$ is correspondingly increased by k_α^p . Hence the Laplace-transformed transition probability is

$$\tilde{p}(\theta, \{y_\alpha\}; q, \{M_\alpha\}) = \sum_{\sigma,\mathbf{k}} c_{\sigma,\mathbf{k}} \exp \left[2\theta\sigma + \sum_{p,\alpha} (y_\alpha - y_{\bar{\alpha}(p,\alpha)}) k_\alpha^p \right]. \quad (42)$$

where the coefficients $c_{\sigma,\mathbf{k}}$ are set to their mean values in a macroscopic state (41)).

A. Entropy and coefficients $c_{\sigma,\mathbf{k}}$ in a macroscopic state defined by q and $\{M_\alpha\}$

Here we use the annealing approximation to estimate the mean values of $c_{\sigma,\mathbf{k}}$ and also of a macroscopic state (q, M_α) . We start by introducing the concept of annealed entropy. Let \mathcal{N} be the number of spin configurations subject to some constraints. In general, it is a function of the disorder realization. The annealed entropy is defined as the logarithm of its disorder average: $s_{\text{ann}} = \ln \langle \mathcal{N} \rangle$. Note that for the correct, quenched, entropy the order of taking a logarithm and disorder average is reversed.

Since in the random hypergraph model all disorder configurations are equally probable, annealed entropy is given as $s_{\text{ann}} = \ln \mathcal{N}_{S,\mathcal{G}} - \ln \mathcal{N}_{\mathcal{G}}$, where $\mathcal{N}_{S,\mathcal{G}}$ is the total number of spin and disorder configurations and $\mathcal{N}_{\mathcal{G}}$ is the number of disorder configurations.

For enumerating all possible disorder configurations we depart slightly from the traditional random hypergraph model. In our model all clauses are ordered (two disorder configurations where any two clauses are permuted are deemed different), clauses can be repeated (the same clause can appear twice), the order of variables in a clause is important (two disorder configurations are different if the order of variables in any clause is changed), and finally, variables can be repeated in a single clause. This change does not alter the underlying physics, since the probability that two identical clauses appear is infinitesimal, and a variable enters a clause twice in at most $O(1)$ clauses, which can be safely neglected. As regards the distinction between the disorders with permuted clauses, this only introduces a combinatorial factor which cancels out. The advantage is that each disorder can be represented as a sequence of M K -tuples of integers from 1 to N .

We will first compute the annealed entropy of a macroscopic state $(q, \{M_\alpha\})$ under additional constraints: we fix the values $c_{\sigma,k}$ and compute the annealed entropy as a function of $q, \{M_\alpha\}, \{c_{\sigma,k}\}$. Recalling that M_α are the numbers of clauses of a given type scaled by N , and the total number of clauses is γN , we obtain the number of joint spin-disorder configurations as a product of the following factors:

- (i) the number of ways to assign types to clauses $(N\gamma)! / \prod_\alpha (NM_\alpha)!$,
- (ii) the number of ways to assign types to variables $N! / \prod_{\sigma,k} (Nc_{\sigma,k})!$,
- (iii) for all p, α , the number of ways to permute the appearance of variables in p -th position of clauses of type α : $(NM_\alpha)! / \prod_{\sigma,k} (k_\alpha^p!)^{Nc_{\sigma,k}}$,

Consequently, the annealed entropy is given by

$$s_{\text{ann}}[\{c_{\sigma,k}\}; q, \{M_\alpha\}] = - \sum_{\sigma,k} c_{\sigma,k} \ln \left[c_{\sigma,k} \prod_{p,\alpha} (k_\alpha^p!) \right] + (K-1) \sum_{\alpha} M_\alpha \ln M_\alpha + \gamma \ln \gamma - \gamma K. \quad (43)$$

In the large N limit we replace $c_{\sigma,k}$ by their annealed averages, i.e., the values that maximize the annealed entropy. In its simplest form, we place no constraints on $c_{\sigma,k}$ except consistency requirements (41). Associating Lagrange multipliers λ and $\ln \mu_\alpha^p$ with these constraints, the expression for the entropy can be rewritten as

$$s_{\text{ann}}[q, \{M_\alpha\}] = \min_{\lambda, \mu_\alpha^p} \left\{ -\lambda q + \sum_{p,\alpha} M_\alpha \ln \frac{M_\alpha}{\mu_\alpha^p} + \ln Z[\lambda, \{\mu_\alpha^p\}] \right\} - \sum_{\alpha} M_\alpha \ln M_\alpha + \gamma \ln \gamma - \gamma K. \quad (44)$$

The values of $c_{\sigma,k}$ are given by

$$c_{\sigma,k} = \frac{1}{Z} e^{\lambda\sigma} \prod_{p,\alpha} (\mu_{\alpha}^p)^{k_{\alpha}^p} / k_{\alpha}^p!, \quad (45)$$

and Z is given by

$$Z = \exp \left(\lambda + \sum_{\alpha} \sum_p \delta[\alpha_p, 1] \mu_{\alpha}^p \right) + \exp \left(-\lambda + \sum_{\alpha} \sum_p \delta[\alpha_p, -1] \mu_{\alpha}^p \right). \quad (46)$$

The values of the Lagrange multipliers λ, μ_{α}^p are related to $q, \{M_{\alpha}\}$ via

$$\frac{\partial \ln Z}{\partial \lambda} = q, \quad (47)$$

$$\mu_{\alpha}^p \frac{\partial \ln Z}{\partial \mu_{\alpha}^p} = M_{\alpha}. \quad (48)$$

From here we obtain the expression for the Lagrange multiplier μ_{α}^p

$$\frac{M_{\alpha}}{\mu_{\alpha}^p} = \frac{1 + \alpha_p q}{2}. \quad (49)$$

Then introducing a new notation

$$\begin{aligned} \mu_{\pm} &= \sum_{p,\alpha} \frac{1 \pm \alpha_p}{2} \mu_{\alpha}^p, \\ M_{\pm} &= \sum_{p,\alpha} \frac{1 \pm \alpha_p}{2} M_{\alpha}, \end{aligned} \quad (50)$$

we obtain

$$Z = e^{\lambda} e^{\mu_{+}} + e^{-\lambda} e^{\mu_{-}}, \quad \mu_{\pm} = \frac{2M_{\pm}}{1 \pm q}. \quad (51)$$

Then the entropy can be rewritten in the following form

$$s_{\text{ann}}[q, \{M_{\alpha}\}] = -\lambda q + M_{+} \ln \frac{1+q}{2} + M_{-} \ln \frac{1-q}{2} + \ln Z - \sum_{\alpha} M_{\alpha} \ln M_{\alpha} + \gamma \ln \gamma - \gamma K. \quad (52)$$

We now use the following equations

$$e^{\lambda} e^{\mu_{+}} = Z \frac{1+q}{2}, \quad e^{-\lambda} e^{\mu_{-}} = Z \frac{1-q}{2} \quad (53)$$

and obtain the expression for the second Lagrange multiplier λ

$$-\lambda q = -\frac{1+q}{2} \ln \frac{1+q}{2} - \frac{1-q}{2} \ln \frac{1-q}{2} - \ln Z + \gamma K. \quad (54)$$

Upon substitution of λ from the above into the expression for s_{ann} (52) we finally obtain the annealed entropy

$$\begin{aligned} s_{\text{ann}}[q, \{M_{\alpha}\}] &= -q \tanh^{-1} q - \ln \frac{\sqrt{1-q^2}}{2} + M_{+} \ln \frac{1+q}{2} + M_{-} \ln \frac{1-q}{2} \\ &\quad - \sum_{\alpha} M_{\alpha} \ln M_{\alpha} + \gamma \ln \gamma. \end{aligned} \quad (55)$$

Also the coefficients $c_{\sigma,k}$ are given by (45),(46) with Lagrange multipliers given in (49) and (54).

B. Effective potential

Consider a factor $\ell(\mathbf{x}) = (\partial f / \partial \Gamma)_\varepsilon$ (25), (26) in the expression (25) for effective potential with $\mathbf{x} \equiv (q, \{M_\alpha\})$. It follows from (26) that to find this factor we need to evaluate the Laplace-transformed probability (40,42) at

$$\theta = \frac{1}{2} \partial s_{\text{ann}} / \partial q, \quad y_\alpha = \frac{1}{2} \partial s_{\text{ann}} / \partial M_\alpha. \quad (56)$$

This is where the Lagrange multipliers come in handy as we can immediately claim that

$$\partial s_{\text{ann}} / \partial q = -\lambda \quad (57)$$

$$\partial s_{\text{ann}} / \partial M_\alpha = \sum_p \ln \frac{M_\alpha}{\mu_\alpha^p} - \ln M_\alpha. \quad (58)$$

Note that in differentiating with respect to M_α above we omitted the constant term. This is permissible since only differences $\partial q_{\text{ann}} / \partial M_\alpha - \partial q_{\text{ann}} / \partial M_{\alpha'}$ appear in Eq. (42). A further refinement is to write

$$\sum_p \ln \frac{M_\alpha}{\mu_\alpha^p} = \sum_p \ln \frac{1 + \sigma_p q}{2} = K \ln \frac{\sqrt{1 - q^2}}{2} + \sum_p \sigma_p \tanh^{-1} q.$$

Using this in the Eqs. (26),(42), we obtain

$$\ell(q, \{M_\alpha\}) = \frac{1}{Z} \sum_{\sigma, \mathbf{k}} \prod_{p, \alpha} \left(\mu_\alpha^p e^{\frac{1}{2} \sum_{p'} (\sigma_{p'} - \sigma'_{p'}) \tanh^{-1} q} \sqrt{\frac{M_{\alpha'}}{M_\alpha}} \right)^{k_\alpha^p} / k_\alpha^p!. \quad (59)$$

Since $\frac{1}{2} \sum_{p'} (\sigma_{p'} - \sigma'_{p'}) \equiv \sigma_p$ (where α' is obtained from α by flipping p -th bit) and also

$$M_\alpha / \mu_\alpha^p = \frac{\sqrt{1 - q^2}}{2} e^{\sigma_p \tanh^{-1} q},$$

the expression is considerably simplified

$$\ell(q, \{M_\alpha\}) = \frac{2}{Z} \exp \left(\frac{2}{\sqrt{1 - q^2}} \sum_{\langle \alpha, \alpha' \rangle} \sqrt{M_\alpha M_{\alpha'}} \right), \quad (60)$$

where the sum is over pairs $\langle \alpha, \alpha' \rangle$ that differ in exactly one position

$$\frac{1}{2} \sum_{p=1}^K |\alpha_j - \alpha'_j| = 1. \quad (61)$$

To evaluate Z we write

$$Z = \frac{2}{\sqrt{1 - q^2}} \sqrt{e^{\mu_+} e^{\mu_-}} = \frac{2}{\sqrt{1 - q^2}} \exp \left(\frac{M_+}{1 + q} + \frac{M_-}{1 - q} \right)$$

and the expression for ℓ becomes

$$\ell(q, \{M_\alpha\}) = \sqrt{1 - q^2} \exp \left(\frac{2 \sum_{\langle \alpha, \alpha' \rangle} \sqrt{M_\alpha M_{\alpha'}}}{\sqrt{1 - q^2}} - \frac{M_+}{1 + q} - \frac{M_-}{1 - q} \right). \quad (62)$$

here M_\pm are given in (50).

We note that the effective potential $f(q, \{M_\alpha\}) = \varepsilon(\{M_\alpha\}) - \Gamma \ell(q, \{M_\alpha\})$ is symmetric with respect to permutation of individual components in $\{M_\alpha\}$ corresponding to different orders of -1's and +1's in the vectorial index α . We look for the minimum of $f(q, \{M_\alpha\})$ using symmetric ansatz

$$M_\alpha = \binom{K}{m}^{-1} \mathcal{M}_m, \quad m = \sum_{p=1}^K \frac{1 - \alpha_p}{2}. \quad (63)$$

where m is the number of -1's in α . Substituting (63) into (62) and rewriting

$$\begin{aligned} \bar{\ell}(q, \{\mathcal{M}_m\}) = & \sqrt{1 - q^2} \exp \left(\frac{2 \sum_{m=0}^{K-1} \sqrt{(m+1)(K-m)} \mathcal{M}_m \mathcal{M}_{m+1}}{\sqrt{1 - q^2}} \right. \\ & \left. - \frac{K\gamma + q \sum_{m=0}^K (K - 2m) \mathcal{M}_m}{1 - q^2} \right). \end{aligned} \quad (64)$$

where we defined $\bar{\ell}(q, \{\mathcal{M}_m\}) \equiv \ell(q, \{M_\alpha\})$. The effective potential is then

$$\bar{f}(q, \{\mathcal{M}_m\}) = \varepsilon(\{\mathcal{M}_m\}) - \Gamma \bar{\ell}(q, \{\mathcal{M}_m\}) \quad (QA), \quad (65)$$

with energy given in (38). In the case of the SA algorithm the corresponding free-energy functional (32) is

$$\bar{f}(q, \{\mathcal{M}_m\}) = \varepsilon(\{\mathcal{M}_m\}) - T \bar{s}(q, \{\mathcal{M}_m\}) \quad (SA), \quad (66)$$

where the entropy function equals

$$\begin{aligned} \bar{s}(q, \{\mathcal{M}_m\}) = & -q \tanh^{-1} q + (\gamma K - 1) \ln \frac{\sqrt{1 - q^2}}{2} \\ & - \left(\sum_{m=0}^K (K - 2m) \mathcal{M}_m \right) \tanh^{-1} q - \sum_{m=0}^K \mathcal{M}_m \ln \frac{\mathcal{M}_m}{\binom{K}{m}}. \end{aligned} \quad (67)$$

If we were to use an even smaller set of macroscopic parameters (e.g. only the energy ε) we can still employ formula (64) with the proviso that unspecified variables should be taken to equal their most likely values, i.e. those that maximize the entropy $\bar{s}(q, \{\mathcal{M}_m\})$ not the landscape $\bar{\ell}(q, \{\mathcal{M}_m\})$. For example, in the case of energy-only landscapes, $\bar{\ell} = \bar{\ell}(\varepsilon)$, the values $q, \{\mathcal{M}_m\}$ that maximize $\bar{s}(q, \{\mathcal{M}_m\})$ for a given energy ε and number of hyperedges γN ($\sum_{m=0}^K \mathcal{M}_m = \gamma$) should be computed and then substituted into the expression for $\bar{\ell}$ (64).

K	1-in-K		K-NAE	
	γ_d	γ_c	γ_d	γ_c
3	—	0.805	—	2.41
4	0.676	0.676	—	5.19
5	0.557	0.609	—	10.7
6	0.475	0.548	19.8	21.8
7	0.416	0.500	34.9	44.0
8	0.371	0.461	61.7	88.4
9	0.335	0.428	109	177
10	0.305	0.400	196	355

TABLE I: Annealing bounds for dynamic (γ_d) and static (γ_c) transition for positive 1-in-K SAT and positive K-NAE SAT for different values of the number of variables in a clause K .

We compute, within the annealing approximation, the point of static transition γ_c (cf. Fig.1), where the entropy of the macroscopic state with zero energy vanishes, $s(0) = 0$, and the dynamic transition γ_d ; for connectivities $\gamma > \gamma_d$ an effective potential (65) exhibits a global bifurcation for some $\Gamma = \Gamma_*$. The resulting values are given in Table I (see also Figs. 2 and 3).

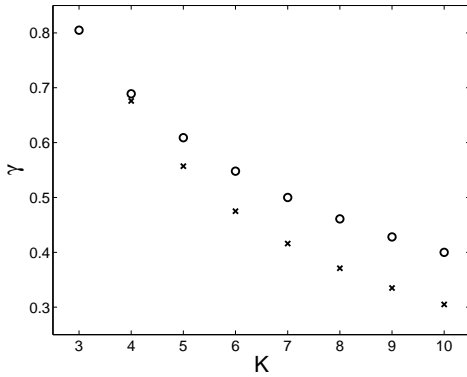


FIG. 2: Static γ_c (circles) and dynamic γ_d (crosses) transition for positive 1-in-K SAT vs K .

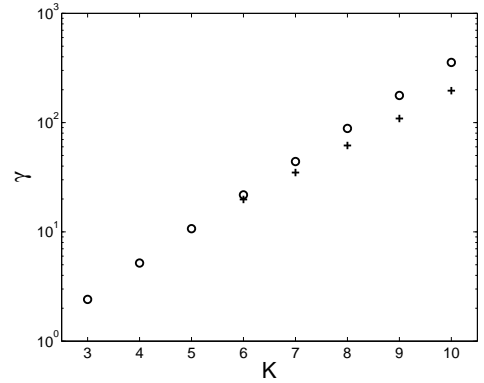


FIG. 3: Static γ_c (circles) and dynamic γ_d (pluses) transition for positive K-NAE SAT vs K .

In Fig. 4 we plot time variations of the landscape parameters, $\mathcal{M}_m = \mathcal{M}_{*m}$, corresponding to the global minimum of the effective potential. In Fig. 5 we plot a time-variation of the scaled ground-state energy g given by the value of the effective potential at its minimum. Singular be-

havior corresponding to the first-order quantum phase transition at certain $\tau = \tau_*$ ($\Gamma = \Gamma_*$) can be clearly seen from the figures. Plots in Figs. 4 and 5 correspond to precisely the static transition $\gamma = \gamma_c$ for the case of $K = 4$ in 1-in-K SAT problem. In the region $\gamma_d < \gamma < \gamma_c$ there are

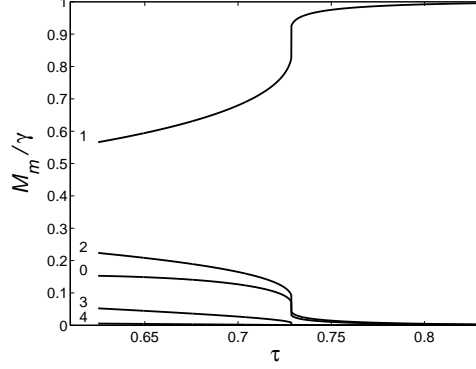


FIG. 4: Plots of the landscape parameters $\mathcal{M}_m = \mathcal{M}_{*m}$ at the global minimum of the effective potential, vs τ for $K = 4$ (1-in-K SAT problem). Curves labelled 0-4 correspond to \mathcal{M}_{*0}/γ through \mathcal{M}_{*4}/γ .

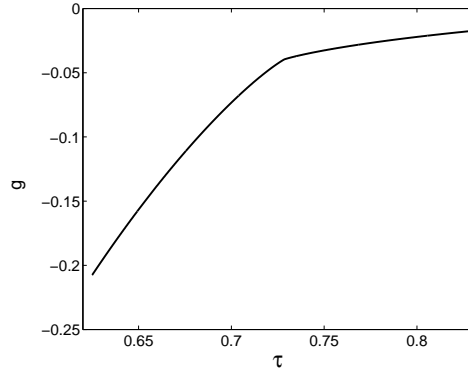


FIG. 5: Scaled energy of adiabatic ground state g vs τ for $K=4$ (1-in-K SAT problem).

exponential (in N) number of solutions to Satisfiability problem but the runtime of the quantum adiabatic algorithm to find any of them also scales exponentially with N . This is a *hard* region for this algorithm. We note, that in the limit of $K \rightarrow \infty$ the annealing approximation becomes exact. Together with the fact that for large K γ_d and γ_c seem to be distinctly different provides evidence that this result (existence of hard region for quantum adiabatic algorithm) is robust.

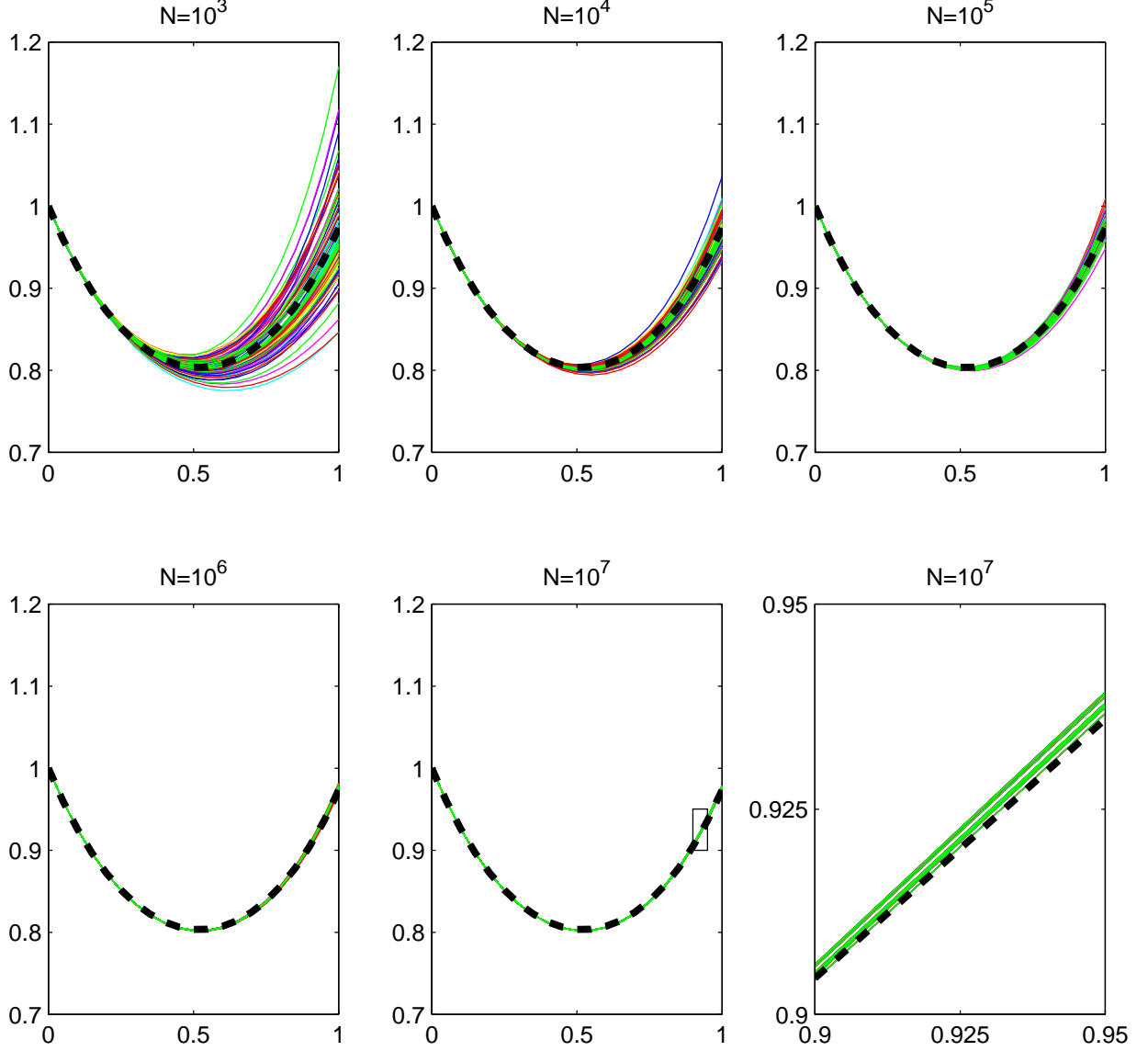


FIG. 6: Results of numerical simulations and their comparison with theory. Depicted are Laplace transforms of M_1 for 1-in-3 SAT. Numerical results: curves that have different colors correspond to different random problem instances; curves of same color correspond to different random bit strings. The dashed black line is a theoretical result based on the annealing approximation. The insets (a)-(e) depict instances with 10^3 , 10^4 , 10^5 , 10^6 , and 10^7 binary variables. Since the error is not recognizable we replot in (f) a magnified section of inset (e). The bit strings were sampled with $q = 0.422$, $\mathcal{M}_0 = 0.048$, $\mathcal{M}_1 = 0.416$, $\mathcal{M}_2 = 0.123$, $\mathcal{M}_3 = 0.013$, corresponding to $M/N = 0.6$. These values correspond to the energy $E_\infty/2$ and they are shifted by 10% from the most likely values of $q, \{\mathcal{M}_m\}$ for this energy (this shift is $\gg N^{1/2}$). We also note that for 1-in-3 SAT numerical simulations give static phase transition at $\gamma_c \approx 0.62$).

VI. UNIVERSALITY PROPERTY FOR TRANSITION PROBABILITIES

Here we study the universal features of the transition probability in (10) for the set of macroscopic variables corresponding to the (normalized) total Ising spin q and numbers of clauses of different types $\{\mathcal{M}_m\}$ (38) (the type of a clause is equal to the number of unit bits involved in the clause). For simplicity, we shall focus in this section on the case $K = 3$ only.

To clarify the above choice of macroscopic variables we consider an auxiliary quantity: a conditional probability distribution of the macroscopic variables $(q, \{\mathcal{M}_m\})$ over the set of all possible configurations σ obtained by flipping r bits of the configuration σ' . The first moments of this distribution corresponding to \mathcal{M}_m ,

$$\mu_m = \binom{N}{r}^{-1} \sum_{\sigma} \delta[d(\sigma' - \sigma), r] M_m(\sigma, \mathcal{I}), \quad m = 0, \dots, K, \quad (68)$$

can be easily computed by counting the number of ways one can flip r bits in configuration σ' to transform a K -bit clause of m' type (i.e., with m' unit bits) into a clause of the m -th type

$$\mu_m = \binom{N}{r}^{-1} \sum_{p, m'=0}^K \mathcal{M}_{m'} \binom{m'}{p} \binom{K-m'}{m-m'+p} \binom{N-K}{r-2p-m+m'}, \quad (69)$$

(here we use the convention $\binom{n}{m} \equiv 0$ for $m < 0$ and $m > n$). In the double sum above values of $\mathcal{M}_{m'}$ are multiplied by the number of possible ways to flip three groups of bits: p unit bits in a clause of m' -type, $p+m-m'$ zero bits of this clause, and $r-2p-m+m'$ bits of the configuration σ' that do not belong to the clause. Similarly, one can show that the first moment corresponding to the variable q equals $q'(1-2r/N)$. It is clear that dependence of the first moments on the ancestor configuration σ' is only via the variables q' , \mathcal{M}'_m for that configuration.

In the limit, $r \gg 1$, the above conditional distribution has a Gaussian form with respect to q and \mathcal{M}_m . Elements of the covariance matrix $\Sigma_{mq}^{m'q'}(\sigma') = \mathcal{O}(r)$, and correspondingly, the characteristic width of the distribution is $\mathcal{O}(r^{1/2})$. For a configuration σ' randomly sampled in the box $(q, \{\mathcal{M}_m\})$ the r.m.s. deviation of the elements of $\Sigma_{mq}^{m'q'}(\sigma')$ from their mean values in the box is $\mathcal{O}(N^{1/2})$. It is clear that in the limit $r \gg N^{1/2}$ the covariance matrix elements can be replaced by their mean values for the macroscopic state $(q, \{\mathcal{M}_m\})$. Therefore in this limit the conditional distribution after r spin flips starting from some macroscopic state depends only on the values of $(q, \{\mathcal{M}_m\})$ in this state (universality property).

One can show that for $r \ll N^{1/2}$ the conditional distribution after r spin flips can be expressed via the distribution (10) with $r = 1$, using a standard convolution rule. However for $r = 1$ the

form of the distribution is non Gaussian and we were not able to establish universality properties in the general form. Instead we performed a series of numerical studies. In Figure 6 we present the results of numerical simulations and the comparison with analytic results within the annealing approximation. One can see that the theory is in very good agreement with experiment.

VII. CONCLUSION

We have formulated an ansatz of landscapes and studied the complexity of the quantum adiabatic algorithm within the annealing approximation and found the existence of a dynamic transition and a hard(exponential) region above that dynamic transition. However, a similar analysis of simulated annealing did not reveal any phase transitions. We explain this as follows. The annealing approximation should fail for sufficiently small energies. It is commonly known that simulated annealing can find suboptimal solutions with very small energies very efficiently, but it takes an exponentially long time to actually reach the ground state. The annealing approximation does not correctly describe very small energies and cannot be used to establish its complexity. Note that we can reconcile this with the fact that the annealing approximation becomes exact in the limit $K \rightarrow \infty$: if the annealing approximation fails for $E \lesssim E_K$ we expect that E_K is decreasing to zero as K increases. However for any finite K , the free energy computed within the annealing approximation is free from any singularities indicative of a phase transition. To study the complexity of simulated annealing one needs to use the tools of spin glass theory, in particular, the replica trick [15–17].

In contrast, in our analysis of the quantum adiabatic algorithm, we observed a first-order phase transition, and, importantly, it happens for energies $E \sim O(E_\infty)$ (where E_∞ is the expected energy at infinite temperature $E_\infty = \frac{1}{2^n} \sum_z E_z$). Moreover, the energies on both sides of the transition, relative to E_∞ seem not to change appreciably with increasing K . Since the annealing approximation for this range of energies can be used, the prediction for the dynamic transition should survive, though the exact numerical values may acquire corrections. We have recomputed the dynamic transition with simplified energy-only landscapes (see Fig. 7). For 1-in- K SAT one can clearly see that the relative correction quickly diminishes. We believe that same happens for K -NAE SAT if sufficiently large K 's are considered. If this indeed holds, it serves as a corroboration that our results are correct numerically for large K . The idea of using energy-only landscapes was present in [7] as well as [21] and [22]. A jump in the time-dependence of the expected energy

value was seen in numerical simulations [8], indicative of first-order phase transition, though a different ensemble was considered (only instances having a unique solution were considered).

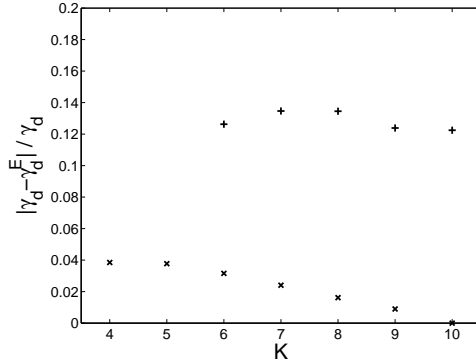


FIG. 7: Relative difference between predictions for the dynamical phase transition point in the case of full (γ_d) and energy-only (γ_d^E) landscapes vs of K for 1-in- K SAT (crosses) and K -NAE SAT (pluses).

We emphasize that the annealing approximation employed in this paper essentially neglects fluctuations due to disorder, and describes the transition as a global bifurcation between two macroscopic states (pure states) and the complexity is due to tunnelling between them. In contrast, spin glass theory predicts the existence of an infinite number of pure states[15]. Secondly, affirming our results for large K ignores the structure of the problem, since that limit corresponds to the so-called random energy model, where one does not expect to do better than $O(2^{N/2})$ via any quantum algorithm. Consequently, the complexity could be determined not by the unique minimum gap, but by a cascade of level repulsion. Numerical studies, however, support the picture with a unique minimum gap. Also, the first-order phase transition occurs for large energies. Although it is absent for small K , we believe that a better approach (as compared to annealing approximation) will reveal it. Moreover, we believe that the order of the transition will remain unchanged, suggesting that the disorder may be irrelevant for the determination of the order of the phase transition and, consequently, for the complexity of the quantum adiabatic algorithm. That is, the exponential complexity is not due to the true combinatorial complexity of the underlying random optimization problem but rather due to peculiarities of the driver term and a particular ensemble of random instances considered. In fact, for a symmetrized variant of the exact cover problem, the same phenomenon was observed – the exponential slowdown – although the problem did not possess any randomness [18, 19]. In fact, a ground state of that problem could be found in $O(N)$ time. However, it was possible to modify the driver term in the annealing Hamiltonian

[20, 23] to circumvent the slowdown. It is quite possible that a similar change of driver term can achieve same goals in present case, although we have not analyzed this scenario. In such a case, one would have to go beyond the annealing approximation to study the complexity.

VIII. ACKNOWLEDGMENTS

This work was supported in part by the National Security Agency (NSA) and Advanced Research and Development Activity (ARDA) under Army Research Office (ARO) contract number ARDA-QC-P004-J132-Y03/LPS-FY2003, we also want to acknowledge the partial support of NASA CICT/IS program.

-
- [1] E. Farhi, J. Goldstone, S. Gutmann, and M. Sipser, arXiv:quant-ph/0001106.
 - [2] E. Farhi, J. Goldstone, S. Gutmann, J. Lapan, A. Lundgren, and D. Preda, *Science* **292**, 472 (2001).
 - [3] S. Lloyd, *Science* **273**, 1073 (1996).
 - [4] W.M. Kaminsky and S. Lloyd, in “Quantum Computing & Quantum Bits in Mesoscopic Systems” (Kluwer Academic, 2003), see also arXiv:quant-ph/0211152.
 - [5] R.M. Karp, in R.E. Miller and J.W. Thatcher, eds. *Complexity of Computer Computations*, Plenum Press, New York, 1972, pp. 85-103.
 - [6] A.M. Childs, E. Farhi, J. Goldstone, and S. Gutmann, arXiv:quant-ph/0012104.
 - [7] T.Hogg, *Phys. Rev. A* **61**, 052311-1 (2000)
 - [8] T. Hogg, arXiv:quant-ph/0206059.
 - [9] Y. Boufkhad, V. Kalapala, and C. Moore, ”The Phase Transition in Positive 1-in-3 SAT”, to be published.
 - [10] G. Semerjian and R. Monasson, *Phys. Rev. E* **67**, 066103 (2003).
 - [11] P. Cheeseman, B. Kanefsky and W.M. Taylor, *Proc. of the International Joint conference on Artificial Intelligence*, **1**, pp. 331-337 (1991).
 - [12] A. Messiah “Quantum Mechanics”, vol. 1 (North-Holland, 1966).
 - [13] S. Kirkpatrick, B. Selman, *Science* **264**, 1297 (1994).
 - [14] *Artificial Intelligence* **81** (1-2) (1996), special issue on Topic, ed. by T. Hogg, B.A. Huberman, and C. Williams.

- [15] M. Mezard, G. Parisi and M.A. Virasoro, eds., *Spin Spin Glass Theory and Beyond* (World Scientific, Singapore, 1987).
- [16] R. Monasson and R. Zecchina, Phys. Rev. Lett **76**, 3881 (1996).
- [17] R. Monasson and R. Zecchina, Phys. Rev. E **56**, 1357 (1997).
- [18] E. Farhi, J. Goldstone, S. Gutmann, arXiv:quant-ph/0201031.
- [19] W. Van Dam, M. Mosca, U. Vazirani, arXiv:quant-ph/0206003.
- [20] E. Farhi, J. Goldstone, S. Gutmann, arXiv:quant-ph/0208135.
- [21] W. Macready, unpublished.
- [22] V. Smelyanskiy, U. Toussaint, D. Timucin, arXiv:quant-ph/0202155.
- [23] A. Boulatov, V. Smelyanskiy, Phys. Rev. A, **68**, issue 6; also quant-ph/0309150.
- [24] M. Mezard, F. Ricci-Tersenghi, R. Zecchina, arXiv:cond-mat/0207140.

APPENDIX A: ON THE NP-COMPLETENESS OF POSITIVE 1-IN- K SAT AND POSITIVE K -NAE-SAT.

We set out to prove that both Positive 1-in- K Sat and K -NAE-Sat are NP-complete. It is straightforward to see that it takes a polynomial time to verify the assignment, so these problems are in NP. We now prove that they are as hard as the Satisfiability problem, which is NP-complete, by showing that any boolean formula can be represented as an instance of these.

1. Positive 1-in- K Sat

A clause of type (x, \dots, x, y) necessarily implies $x = 0$ and $y = 1$; hence we can represent constants 0 and 1. A clause of type $(0, \dots, 0, x, y)$ implies $x = \neg y$. Finally, a clause of type $(0, \dots, 0, x, y, z)$ is equivalent to a 3-clause (x, y, z) so that we can restrict ourselves to $K = 3$ without losing generality.

For $K = 3$, immediately observe that three clauses $(x, z, u')(y, z, u'')(u, u', u'')$ with free variables u, u', u'' implies $z = \neg(x \wedge y)$. This basic building block is in fact sufficient to build any boolean formula, as a result, any boolean formula can be cast as an 1-in- K SAT formula.

2. Positive K -NAE-Sat

A clause of type (x, \dots, x, y) necessarily implies $x = \neg y$, and (x, \dots, x, y, z) is equivalent to (x, y, z) so we once again restrict ourselves to $K = 3$. In contrast to 1-in- K problem, we shall require a non-trivial representation of *false* or *true*. We will use *pairs* of variables to denote variables of the boolean formula. Pairs 00 or 11 will represent value *false* and pairs 01 or 10 will represent *true*.

The next building block, $(x, y, t)(y, z, t)(z, x, t)$ ensures that $t = 1$ if the majority of x, y, z are 0 and $t = 0$ if the majority are 1. We shall use a shorthand $f(t; x, y, z)$ to denote this. The expression $f(z_1; x_1, y_1, y_2)f(z_2; x_2, y_1, y_2)$ then ensures $z = x \wedge y$ where x, y, z are represented as pairs x_1x_2, y_1y_2, z_1z_2 as indicated above. The operation of negation is trivial to represent: if $x \equiv x_1x_2$ then $\neg x \equiv (\neg x_1)x_2$. These two are sufficient to construct any boolean formula.

APPENDIX B: NEXT ORDER APPROXIMATION FOR LANDSCAPES

A better approximation for the values of critical clause-to-variable ratios can be obtained if we specify the constraint that the distribution of vertex degrees be Poisson (as it is supposed to be in a random hypergraph [24]). To be precise, we specify that

$$\sum_{\sigma, \mathbf{k}} c_{\sigma, \mathbf{k}} \prod_p \delta \left(\sum_{\alpha} k_{\alpha}^p - k_p \right) = c_{\{k_p\}} \equiv \frac{\prod_p \gamma^{k_p}}{\prod_p k_p!} e^{-\gamma K}. \quad (\text{B1})$$

Consequently, with this constraint the following expression for $c_{\sigma, \mathbf{k}}$ is obtained:

$$c_{\sigma, \mathbf{k}} = c_{\{k_p\}} \frac{e^{\lambda s} \prod_p [k_p! \prod_{\alpha} (\mu_{\alpha}^p)^{k_{\alpha}^p} / k_{\alpha}^p!]}{Z_{\{k_p\}}}, \quad (\text{B2})$$

where we use

$$Z_{\{k_p\}} = e^{\lambda} \prod_p \left(\sum_{\alpha} \delta(\alpha_p - 1) \mu_{\alpha}^p \right)^{k_p} + e^{-\lambda} \prod_p \left(\sum_{\alpha} \delta(\alpha_p + 1) \mu_{\alpha}^p \right)^{k_p}. \quad (\text{B3})$$

Annealed entropy can be rewritten in the form

$$s_{\text{ann}}[q, \{M_{\alpha}\}] = \min_{\lambda, \mu_{\alpha}^p} \left\{ -\lambda q + \sum_{p, \alpha} M_{\alpha} \ln \frac{M_{\alpha}}{\mu_{\alpha}^p} + \ln Z[\lambda, \mu_{\alpha}^p] \right\} - \sum_{\alpha} M_{\alpha} \ln M_{\alpha} + \gamma \ln \gamma - \gamma K,$$

where $\ln Z$ is given by

$$\ln Z = \sum_{\{k_p\}} c_{\{k_p\}} \ln Z_{\{k_p\}}.$$

The equations relating q , $\{M_\alpha\}$ and λ , $\{\mu_\alpha^p\}$ are given in (47),(48).

Similarly to Sec. VB we will use the notation (50). Since $\ln Z$ depends only on λ and μ_\pm , $\partial \ln Z / \partial \mu_\alpha^p$ depends only on σ_p . Therefore, $M_\alpha / \mu_\alpha^p = M_{\sigma_p} / \mu_{\sigma_p}$. Correspondingly,

$$s_{\text{ann}}[q, \{M_\alpha\}] = \min_{\lambda, \mu_\pm} \left\{ -\lambda q + M_+ \ln \frac{M_+}{\mu_+} + M_- \ln \frac{M_-}{\mu_-} + \ln Z \right\} - \sum_\alpha M_\alpha \ln M_\alpha + \gamma \ln \gamma - \gamma K$$

For convenience, we introduce new variables

$$\mu_\pm = \mu e^{\pm h}. \quad (\text{B4})$$

We then readily obtain

$$\ln Z = \gamma \ln \mu + \sum_k c_k \ln[2 \cosh(\lambda + kh)],$$

(where $k = \sum_p k_p$ and $c_k = \frac{(\gamma K)^k}{k!} e^{-\gamma K}$) and μ drops out of the expression for s_{ann} altogether:

$$\begin{aligned} s_{\text{ann}}[q, \{M_\alpha\}] = \min_{\lambda, h} & \left\{ -\lambda q - (M_+ - M_-)h + \sum_k c_k \ln[2 \cosh(\lambda + kh)] \right\} \\ & - \sum_\alpha M_\alpha \ln M_\alpha + M_+ \ln M_+ + M_- \ln M_- + \gamma \ln \gamma - \gamma K. \end{aligned} \quad (\text{B5})$$

It is easy to see from this expression what the equations for λ, h are:

$$\begin{aligned} \sum_k c_k \tanh[\lambda + kh] &= q, \\ \sum_k k c_k \tanh[\lambda + kh] &= M_+ - M_-. \end{aligned} \quad (\text{B6})$$

We now turn our attention to the function $\ell(q, \{M_\alpha\})$ given by (42) with θ and y_α evaluated from Eqs. (56),(58). The computation of $e^{y_\alpha - y_{\alpha'}}$ yields

$$e^{y_\alpha - y_{\alpha'}} = \left(\sqrt{\frac{M_+}{M_-}} \sqrt{\frac{\mu_-}{\mu_+}} \right)^{\sigma_p} \sqrt{\frac{M_{\alpha'}}{M_\alpha}}. \quad (\text{B7})$$

Multiplied by μ_α^p this becomes

$$\mu_\alpha^p e^{y_\alpha - y_{\alpha'}} = \frac{\sqrt{M_\alpha M_{\alpha'}}}{\sqrt{M_+ M_-}} \mu. \quad (\text{B8})$$

The expression for $\ell(q, \{M_\alpha\})$ can be written in the form (cf. (59))

$$\ell(q, \{M_\alpha\}) = \sum_{\{k_p\}} \frac{C_{\{k_p\}}}{Z_{\{k_p\}}} \sum_{\sigma, \mathbf{k}}' e^{\lambda s + 2xs} \prod_p \left[k_p! \prod_\alpha (\mu_\alpha^p e^{y_\alpha - y_{\alpha'}})^{k_\alpha^p} / k_\alpha^p! \right],$$

with the internal sum running over \mathbf{k} consistent with a set of $\{k_p\}$ (B1). Substituting the quantities defined above this becomes

$$\ell(q, \{M_\alpha\}) = \sum_{\{k_p\}} c_{\{k_p\}} \frac{\sum_\sigma \prod_p \left(\mu \sum_\alpha \delta(\alpha_p - \sigma) \frac{\sqrt{M_\alpha M_{\alpha'}}}{\sqrt{M_+ M_-}} \right)^{k_p}}{Z_{\{k_p\}}}. \quad (\text{B9})$$

After some transformations we finally obtain

$$\ell(q, \{M_\alpha\}) = \sum_k c_k \frac{\left(\frac{\sum_{\langle \alpha, \alpha' \rangle} \sqrt{M_\alpha M_{\alpha'}}}{\sqrt{M_+ M_-}} \right)^k}{\cosh[\lambda + kh]}. \quad (\text{B10})$$

where λ, h are given by (50),(B6). Using symmetric ansatz (63) it is straightforward to calculate from (B10) the restricted function $\bar{\ell}(q, \{\mathcal{M}_m\})$ (cf. (64)). We must note however, that although this represents a next-order improvement over annealing approximation, the relative changes in γ_c and γ_d computed with this improved approximation are nearly imperceptible ($\sim 10^{-4}$).